# Numerical Analysis (6/7)
## Linear systems

University of Luxembourg - 2024

Master in Mathematics

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## Outline

1. Introduction
2. LU decomposition
3. QR decomposition
4. Iterative methods
5. Summary


# 1. Introduction

# Overview of the content

We already encountered linear system in different situations

- interpolation (global and splines),
- least-square data fit (normal equations),
- finite difference methods (tridiagonal system),

In general, almost all PDE problems (even non-linear ones) require to solve at some point a linear system of the form

$$Ax = b, \quad \text{of size } N \times N$$

We will study two kind of resolution methods

1. Direct methods,
2. Iterative methods,

The "best" method for solving $A$ quickly and accurately is problem dependent.

# Overview of the content

There are two families of methods

1. Direct methods : where we obtain the exact solution (up to round-off errors) in a finite number of operations
   - LU factorization, $A = LU$
   - QR factorization (see exercise), $A = QR$
   - Singular value decomposition (SVD), $A = U\Sigma V^*$
2. Iterative methods : they consist in building a sequence of vectors $x^k$ converging towards the solution $x$. It is stopped after a finite number of iterations $k$ chosen in such a way that $x^k$ is close enough to $x$
   - Fixed point iteration: Jacobi, Gauss-Seidel, SOR
   - Krylov subspace: conjugate gradient, GMRES, ...

# Important remarks

## Remarks

- we never use the Cramer's formulas

$$A^{-1} = \frac{\text{com}A^T}{\det A}$$

since they need to compute determinants which is a highly computationally expensive task (too much elementary operations)

- we never compute $A^{-1}$ to solve $Ax = b$.
Numerically, this is in the other way : the computation of $A^{-1}$, and also $\det A$, are a by-product of the solution to the linear systems.

To compute $A^{-1}$ we may solve

$$\{Ax_i = e_i,\ i = 1, ..., n\}$$

where $e_i$ is $i$-th vector of the $\mathbb{R}^n$ canonical basis. The $i$-th column of $A^{-1}$ is $x_i$.


# 2. LU factorization

# Linear system that is easy to solve

A general idea is to try to transform the linear systems into an easier one

## Diagonal matrix

all the elements are zero expect the ones on the main diagonal

$$A = \begin{bmatrix} a_1 & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & a_n \end{bmatrix}$$

If $A$ is invertible then all the $a_i$ are non zero and the solution of $Ax = b$ is trivial.
If $x = (x_1, ..., x_n)$ and $b = (b_1, ..., b_n)$, we have

$$x_i = \frac{b_i}{a_i},\ i = 1, ..., n$$

# Upper (or lower) triangular matrices

All the elements below (or above) the main diagonal are zeros, i.e. $a_{ij} = 0$ for $i > j$ or $(i < j)$

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ 0 & \ddots & & \vdots \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & a_{nn} \end{bmatrix}$$

In this case, the linear system writes

$$\begin{cases} a_{11}x_1 + a_{12}x_2 + \ldots + a_{1n}x_n = b_1 \\ a_{22}x_2 + \ldots + a_{2n}x_n = b_2 \\ \vdots \\ a_{n-1,n-1}x_{n-1} + a_{n-1,n}x_n = b_{n-1} \\ a_{nn}x_n = b_n \end{cases}$$

We always use a direct method for the solution, called backward (forward) elimination process

# Backward substitution

Exercise 1

we start by solving the last equation ; we substitute the result $x_n$ in the previous equation, which provides $x_{n-1}$, and so on...

$$\begin{cases} x_n = b_n / a_{nn} \\ x_{n-1} = (b_{n-1} - a_{n-1,n} x_n) / a_{n-1,n-1} \\ \vdots \\ x_i = (b_i - a_{i,n} x_n - a_{i,n-1} x_{n-1} - \ldots - a_{i,i+1} x_{i+1}) / a_{ii} \\ \vdots \end{cases}$$

(the triangular matrix $A$ is always assumed to be invertible so $a_{ii} \neq 0$ for all $i$)

## Cost of the backward procedure

The computation of $x_i$ requires: 1 division, $n - i$ multiplications, $n - i$ additions.
Therefore it needs a total of $n$ divisions, $\frac{n(n-1)}{2}$ multiplications, $\frac{n(n-1)}{2}$ additions, which is about $\mathcal{O}(n^2)$ elementary operations.

# Upper (or lower) triangular matrices

## Remarks

- the same algorithm is used for lower triangular systems, which is called forward substitution,
- we will see that a cost of $\mathcal{O}(n^2)$ is cheap compared to the cost of more general direct methods,
- the idea is then to transform more complicated systems into such a triangular form

# Gauss elimination

The Gauss method is a general method for solving a linear system

$$Ax = b$$

where $A$ is an invertible matrix (not necessarily square). It needs 3 steps :

1. a procedure called "elimination process" which corresponds to find an invertible matrix $M$ such that the matrix $MA$ is upper triangular
2. Compute the vector $Mb$
3. Solve the easier linear system

$$MAu = Mb$$

where the matrix $MA$ is upper triangular and can be solved by the backward elimination process.

# Description of the first step

We will perform elimination thanks to row operations, namely we are allowed to

1. Multiplying a row by a value,
2. Adding one row to another row,
3. Exchanging two rows with each other.

Let $A = (a_{i,j}), \quad i \in [\![1, n]\!],\ j \in [\![1, n]\!]$

- at least one of the coefficients $a_{i,1},\ i \in [\![1, n]\!]$ of the first column $A$ is not zero, otherwise the matrix would not be invertible
- we choose one of these nonzero coefficients, called the first pivot of the elimination.
- we exchange the row of the pivot with the first row which in a matrix notation is equivalent to left multiply $A$ by a specific matrix.

Row exchange can be seen as a matrix operation

# Illustration of the algorithm

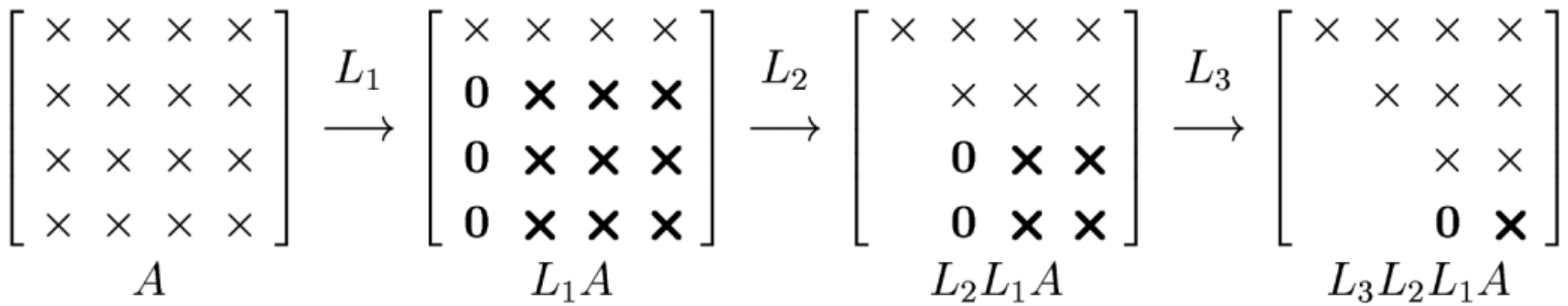



Figure: Illustration of the Gaussian elimination algorithm. From *Trefeten and Bau, Numerical Linear Algebra III*(1997)

# Theorem

## Theorem: $LU$ factorisation

Let $A = (a_{i,j})$ be a square matrix of size $n$ such as all the submatrices

$$\Delta_k = \begin{pmatrix} a_{1,1} & \cdots & a_{1,k} \\ \vdots & & \vdots \\ a_{k,1} & \cdots & a_{k,k} \end{pmatrix} \quad k \in [\![1, n]\!]$$

are invertible. Then there is a unique lower triangular matrix $L = (l_{i,j})$ with $l_{i,i} = 1$ for all $i \in [\![1, n]\!]$ and an upper triangular matrix $U$ such as

$$A = LU$$

Remark: if we allow row permutations (a pivoting startegy), we have that any square matrix admits a PLU decomposition such that

$$PA = LU$$

Remark 2: this is not obvious, because we may apply a permutation at each $k$th-step !

# Example (hands on)

Exercise 2

$$A = \begin{pmatrix} 2 & 4 & 3 & 5 \\ -4 & -7 & -5 & -8 \\ 6 & 8 & 2 & 9 \\ 4 & 9 & -2 & 14 \end{pmatrix}$$

$$A = \underbrace{\begin{pmatrix} 1 & & & \\ -2 & 1 & & \\ 3 & -4 & 1 & \\ 2 & 1 & 3 & 1 \end{pmatrix}}_{L} \cdot \underbrace{\begin{pmatrix} 2 & 4 & 3 & 5 \\ 0 & 1 & 1 & 2 \\ 0 & 0 & -3 & 2 \\ 0 & 0 & 0 & -4 \end{pmatrix}}_{U}$$

# Choice of the pivot

- at the beginning of the $k$th step of the elimination process, theoretically one can choose any coefficient $a_{i,k}^k$ which is nonzero ($i \in [\![k, n]\!]$)
- in particular, if $a_{k,k}^k$ is nonzero we can choose it as the pivot (and then $P_k = I$)
- however, this way of proceeding can lead to round-off errors and an incorrect solution

# Choice of the pivot

**Example**

Let us consider the system

$$\begin{pmatrix} 10^{-4} & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 1 \\ 2 \end{pmatrix}$$

The exact solution is

$$x_1 = \frac{10000}{9999} \simeq 1, \quad x_2 = \frac{9998}{9999} \simeq 1$$

- let us assume that the computations are realized up to 3 digits
- first case:

$$\begin{array}{cc|c} 10^{-4} & 1 & 1 \\ 1 & 1 & 2 \end{array} \qquad \begin{array}{cc|c} 10^{-4} & 1 & 1 \\ 0 & -9.99\ 10^{3} & -9.99\ 10^{3} \end{array}$$

$$x_2 = 1 \quad \text{and} \quad x_1 = 0!$$

# Choice of the pivot

**Example**

Let us consider the system

$$\begin{pmatrix} 10^{-4} & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 1 \\ 2 \end{pmatrix}$$

- second case:

$$\begin{array}{cc|cc|c|c} 1 & 1 & 2 & 1 & 1 & 2 \\ 10^{-4} & 1 & 1 & 0 & 9.99\ 10^{-1} & 9.99\ 10^{-1} \end{array}$$

$$x_2 = 1 \quad \text{and} \quad x_1 = 1$$

- the rule is to rather use the pivot which corresponds to the coefficient with largest amplitude
- The partial pivot strategy : we determine the element $a_{i,k}^k$ (or one of the elements $a_{i,k}^k$) such that $k \leq i \leq n$ and

$$\left|a_{i,k}^k\right| = \max_{k \leq j \leq n} \left|a_{j,k}^k\right| .$$

# Cost of Gauss method

- To get from $A_k$ to $A_{k+1}$ we need

$$n-k \text{ divisions, } (n-k)(n-k+1) \text{ additions and multiplications}$$

- leading a total of

$$\frac{n(n-1)}{2} \text{ divisions, } \frac{n^3-n}{3} \text{ multiplications and additions}$$

or

$$\frac{4n^3+3n^2-7n}{6} \text{elementary operations}$$

- we need to add the $n^2$ elementary operations for the forward substitution.
- When $n$ is large, the terms scaling in $n^2$ and $n$ small compared to $n^3$ and the global number of operations is around

$$\frac{2n^3}{3}$$

# Remarks

- a cost of $\mathcal{O}(n^3)$ is huge for large linear systems !
- the numerical stability of Gaussian elimination, even with partial pivoting, is not obvious. A proper *backward analysis* is required: the key relies in the amplification of the entries $a_{k,k}^k$ during the elimination process, called the growth factor

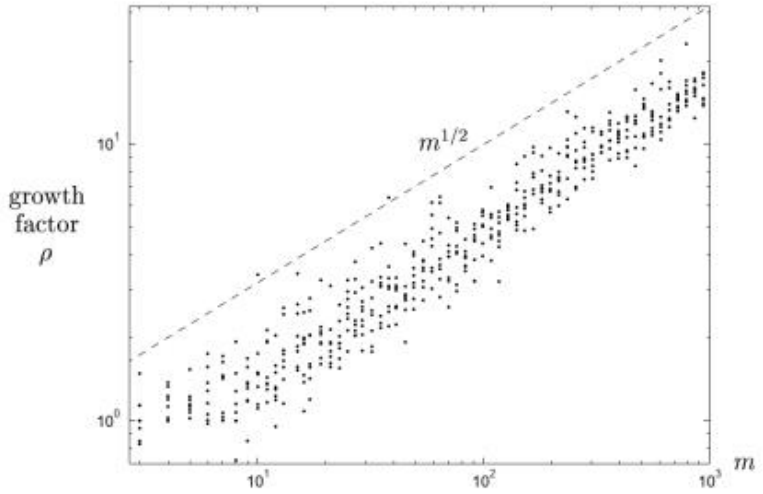



Figure 22.1. *Growth factors for Gaussian elimination with partial pivoting applied to* 496 *random matrices (independent, normally distributed entries) of various dimensions. The typical size of* $\rho$ *is of order* $m^{1/2}$*, much less than the maximal possible value* $2^{m-1}$.

Figure: From *Trefeten and Bau, Numerical Linear Algebra III*(1997)

# LU factorization pseudo-code

Exercise 2

## LU pseudo-code without pivoting

Initialize $L$ to an identity matrix of dimension $n \times n$ and $U = A$

For $i = 1 \cdots n$
    For $j = (i+1), \cdots n$
        $\ell_{ji} = u_{ji} / u_{ii}$
        $U_j \rightarrow U_j - \ell_{ji} U_i$
return $L, U$

# LU factorization pseudo-code with pivoting

Exercise 3

## LU pseudo-code with simple pivoting

Initialize $L$ to an identity matrix of dimension $n \times n$ and $U = A$

For $i = 1 \cdots n$
  Let $k = i$
  While $u_{ii} = 0$
    Swap row $U_i$ with row $U_{k+1}$
    Swap row $P_i$ with row $P_{k+1}$
    $k = k + 1$
  For $j = (i + 1), \cdots n$
    $\ell_{ji} = u_{ji} / u_{ii}$
    $U_j \rightarrow U_j - \ell_{ji} U_i$
return $L, U$

Remark: the partial pivoting strategy consists in looking for the max $u_{k,i}$ value over all remaining rows at the $k$-th step, and then swapping rows

# Solving a linear system with LU factorization

- we would like to solve

$$Ax = b \iff LUx = b$$

- Once we have $L$ and $U$, we first solve

$$Ly = b$$

with backward substitution (we have $y = Ux$)

- then we solve

$$Ux = y$$

with forward substitution

# Factorization cost

- $LU$ factorisation has the same cost as Gaussian elimination, that is $\frac{2n^3}{3}$ elementary operations
- we need to add forward-backward substitution which adds $n^2$ elementary operations
- Once the $LU$ factorization is done, we can treat multiple right-hand sides $b$
- For positive-definite matrices, one can write $A = LL^T$, which reduces the cost by a factor 2. The associated method is called Cholesky factorization
- When the matrix contains many zeros, the computational cost can be highly reduced. We talk about sparse matrices

# A few words on sparse matrices

The discretization of many engineering problems requires to solve linear systems with only a few non-zero entries (nz)

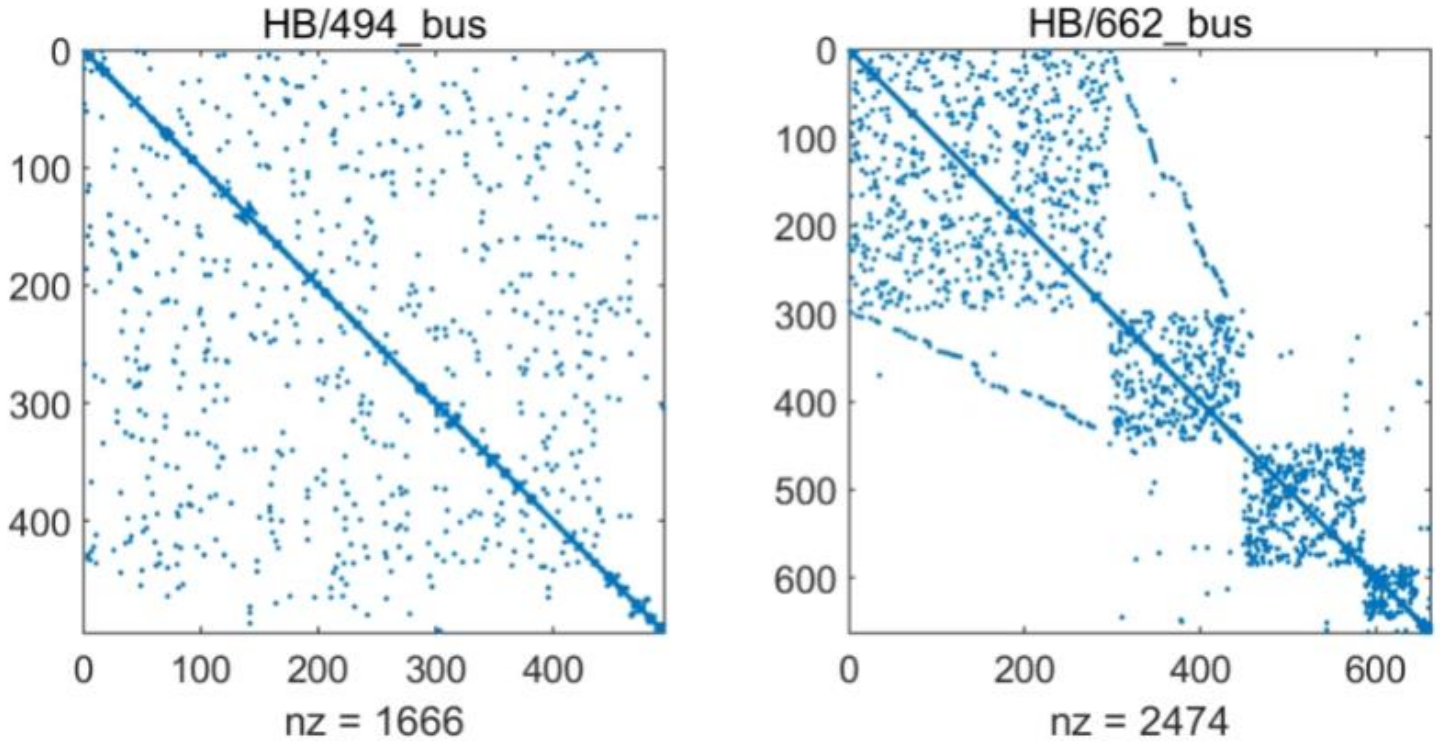



Figure: Example of sparsity patterns for two symmetric positive definite matrices. Nonzero elements are indicated by dots. From Nick Higham blog

# A few words on sparse matrices

**Bandwidth of a matrix**

The bandwidth of a matrix $A$ is the smallest non-negative integer $m$ such that

$$a_{ij} = 0, \quad \text{for } |i - j| > m$$

The LU decomposition does not increase the bandwidth !
The cost of LU factorization reduces to $\mathcal{O}(m^2 N)$

**Example**

Gaussian elimination for a tridiagonal matrix (Thomas algorithm) - $\mathcal{O}(N)$ operations !

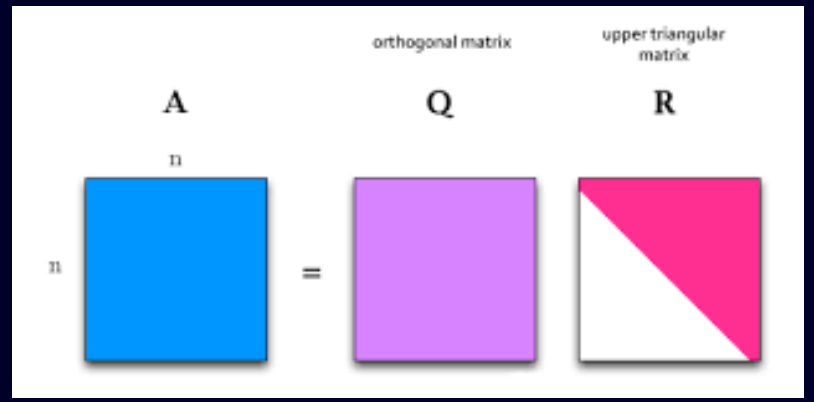
Moreover *reordering* strategies can be highly beneficial and highlight a sparsity pattern.

Special libraries are designed for sparse matrices and are routinely used in the industry: `MUMPS`, `pardiso`, `superLU`, `UMFPACK`, ...


# 3. QR decomposition

# QR decomposition (for square matrices)

- **Definition:**
  - Any $n \times n$ matrix $A$ can be decomposed into:
    - $\boldsymbol{Q}$: A matrix with orthonormal columns ($Q^T Q = I$)
    - $\boldsymbol{R}$: An upper triangular matrix




- **Steps for Decomposition:**
  - **Classical Approach**: Gram-Schmidt orthogonalization process.
  - **Alternative Methods**: Householder reflections or Givens rotations

- **Applications:** Often used in least-squares problems and eigenvalue problems.

# QR decomposition

Consider the Gram–Schmidt process applied to the columns of the full column rank matrix $A = \begin{bmatrix} \mathbf{a}_1 & \cdots & \mathbf{a}_n \end{bmatrix}$, with inner product $\langle \mathbf{v}, \mathbf{w} \rangle = \mathbf{v}^{\mathsf{T}} \mathbf{w}$ (or $\langle \mathbf{v}, \mathbf{w} \rangle = \mathbf{v}^{\dagger} \mathbf{w}$ for the complex case).

Define the projection:

$$\operatorname{proj}_{\mathbf{u}} \mathbf{a} = \frac{\langle \mathbf{u}, \mathbf{a} \rangle}{\langle \mathbf{u}, \mathbf{u} \rangle} \mathbf{u}$$

then:

$$\begin{aligned}
\mathbf{u}_1 &= \mathbf{a}_1, & \mathbf{e}_1 &= \frac{\mathbf{u}_1}{\|\mathbf{u}_1\|} \\
\mathbf{u}_2 &= \mathbf{a}_2 - \operatorname{proj}_{\mathbf{u}_1} \mathbf{a}_2, & \mathbf{e}_2 &= \frac{\mathbf{u}_2}{\|\mathbf{u}_2\|} \\
\mathbf{u}_3 &= \mathbf{a}_3 - \operatorname{proj}_{\mathbf{u}_1} \mathbf{a}_3 - \operatorname{proj}_{\mathbf{u}_2} \mathbf{a}_3, & \mathbf{e}_3 &= \frac{\mathbf{u}_3}{\|\mathbf{u}_3\|} \\
&\vdots & &\vdots \\
\mathbf{u}_k &= \mathbf{a}_k - \sum_{j=1}^{k-1} \operatorname{proj}_{\mathbf{u}_j} \mathbf{a}_k, & \mathbf{e}_k &= \frac{\mathbf{u}_k}{\|\mathbf{u}_k\|}
\end{aligned}$$

We can now express the $\mathbf{a}_i$s over our newly computed orthonormal basis:

$$\begin{aligned}
\mathbf{a}_1 &= \langle \mathbf{e}_1, \mathbf{a}_1 \rangle \mathbf{e}_1 \\
\mathbf{a}_2 &= \langle \mathbf{e}_1, \mathbf{a}_2 \rangle \mathbf{e}_1 + \langle \mathbf{e}_2, \mathbf{a}_2 \rangle \mathbf{e}_2 \\
\mathbf{a}_3 &= \langle \mathbf{e}_1, \mathbf{a}_3 \rangle \mathbf{e}_1 + \langle \mathbf{e}_2, \mathbf{a}_3 \rangle \mathbf{e}_2 + \langle \mathbf{e}_3, \mathbf{a}_3 \rangle \mathbf{e}_3 \\
&\vdots \\
\mathbf{a}_k &= \sum_{j=1}^{k} \langle \mathbf{e}_j, \mathbf{a}_k \rangle \mathbf{e}_j
\end{aligned}$$

where $\langle \mathbf{e}_i, \mathbf{a}_i \rangle = \|\mathbf{u}_i\|$. This can be written in matrix form:

$$A = QR$$

where:

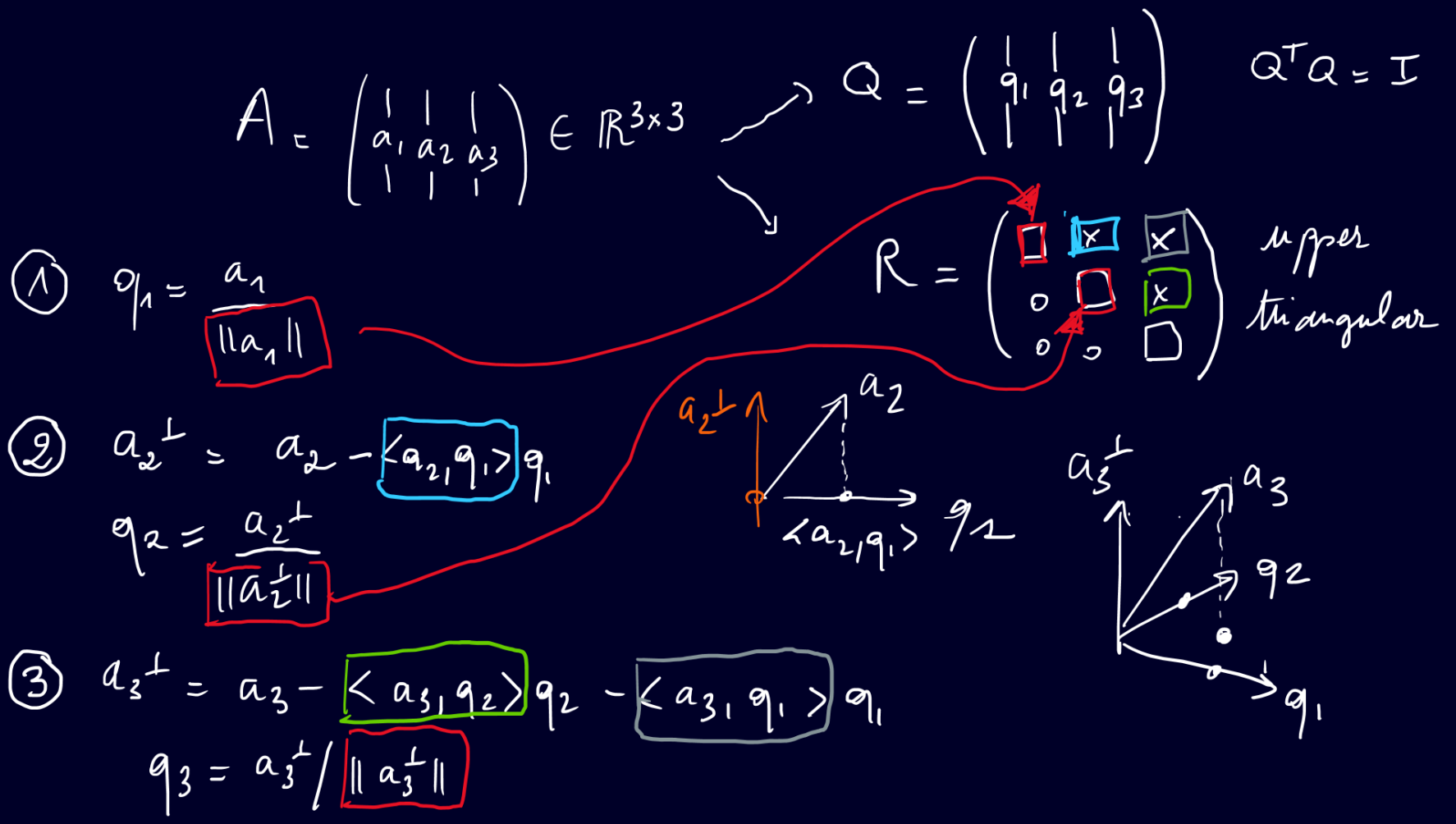
$$Q = \begin{bmatrix} \mathbf{e}_1 & \cdots & \mathbf{e}_n \end{bmatrix}$$

and

$$R = \begin{bmatrix} \langle \mathbf{e}_1, \mathbf{a}_1 \rangle & \langle \mathbf{e}_1, \mathbf{a}_2 \rangle & \langle \mathbf{e}_1, \mathbf{a}_3 \rangle & \cdots & \langle \mathbf{e}_1, \mathbf{a}_n \rangle \\ 0 & \langle \mathbf{e}_2, \mathbf{a}_2 \rangle & \langle \mathbf{e}_2, \mathbf{a}_3 \rangle & \cdots & \langle \mathbf{e}_2, \mathbf{a}_n \rangle \\ 0 & 0 & \langle \mathbf{e}_3, \mathbf{a}_3 \rangle & \cdots & \langle \mathbf{e}_3, \mathbf{a}_n \rangle \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \langle \mathbf{e}_n, \mathbf{a}_n \rangle \end{bmatrix}.$$

https://en.wikipedia.org/wiki/QR_decomposition

# QR algorithm




- The QR decomposition is based on a Gram-Schmidt orthogonalization process

# Example (hands on)

$$A = \begin{pmatrix} 1 & 3 \\ 1 & -1 \end{pmatrix}$$

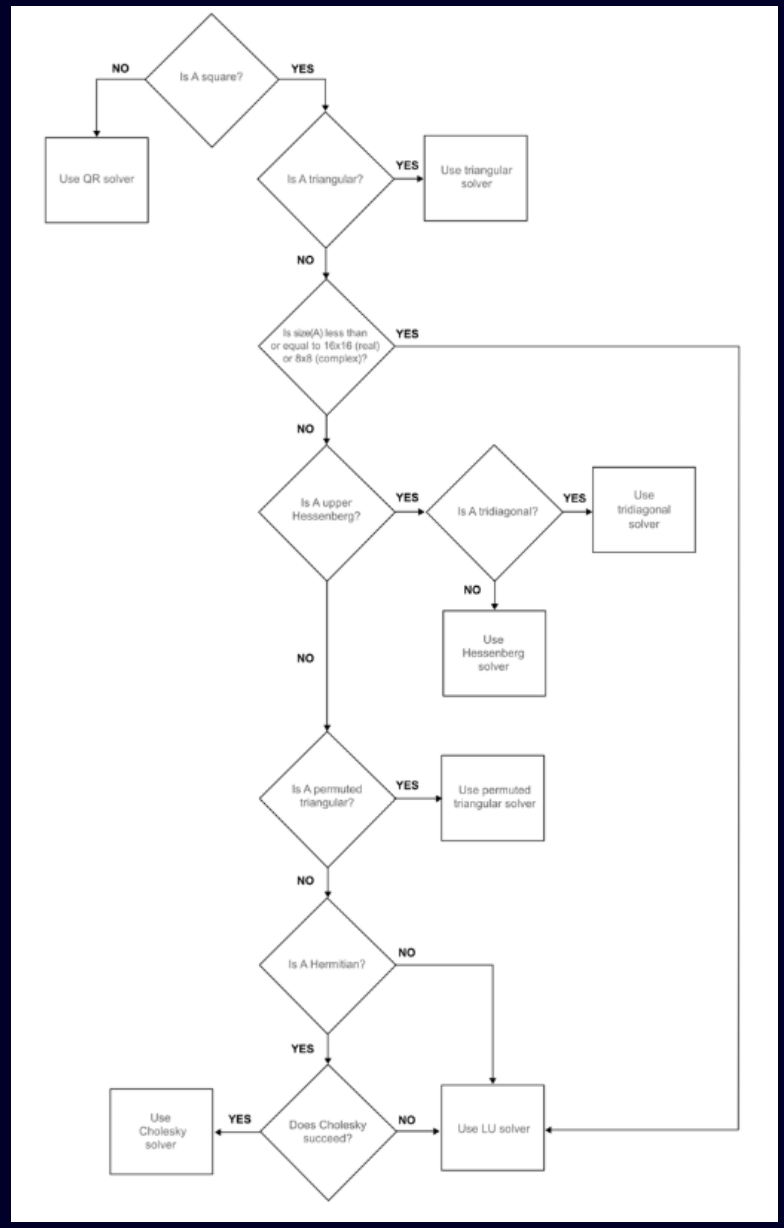
$$Q = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{pmatrix}$$

$$R = \begin{pmatrix} \sqrt{2} & \sqrt{2} \\ 0 & 2\sqrt{2} \end{pmatrix}$$

# Backslah in Matlab

https://www.mathworks.com/help/matlab/ref/double.mldivide.html

- **Decision tree**
  - Use QR solver for non square matrices
  - Use Cholesky for square symmetric matrices
  - Use LU otherwise




Exercise 4


# 3. Iterative solvers

# Introduction

Given an invertible matrix $A$ inversible, we would like to determine the solution to the linear system

$$Au = b$$

by an iterative method. We focus the analysis on square matrices.
we would like to build a sequence of vectors $(u_k)_{k\geq 0}$ such that

1. $$\begin{cases} u_{k+1} = Bu_k + c, & \forall\ k \geq 0 \\ u_0 \text{ given} \end{cases}$$

   where the matrix $B$ and the vector $c$ are defined from $A$ and $b$
2. the sequence $(u_k)_{k\geq 0}$ converges and the limit $u$ is the solution to the linear system.

Remark: we solve the system only computing matrix-vector products at each iteration

# Some basic notions

## Convergence of an iterative method

These statements are equivalent :

- the iterative method converges, that is $(u_k)_{k\geq 0} \to u$ for any initial $u_0$
- the spectral radius is less than 1

$$\rho(B) < 1$$

- for at least one matrix norm $\|.\|$

$$\|B\| < 1$$

Remark: the iterative method is a fixed-point approach for

$$\begin{array}{rcl} f : \mathbb{C}^n & \to & \mathbb{C}^n \\ v & \to & Bv + c \end{array}$$

which is a contraction when $\|B\| < 1$

# Some induced matrix norms

- 2-norm

$$\|A\|_2 = \sqrt{\rho(A^T A)}$$

  with $\rho(B) = \max\{|\lambda_i|, \lambda_i \text{ is an eigenvalue of } B\}$

- $\infty$-norm

$$\|A\|_\infty = \max_{1 \le i \le m} \sum_{j=1}^{n} |a_{ij}|$$

- 1-norm

$$\|A\|_1 = \max_{1 \le j \le n} \sum_{i=1}^{m} |a_{ij}|$$

Remark: the 2-norm is harder to compute in practice

# Speed of convergence

Let $\|.\|$ be a matrix norm and $u$ such that

$$u = Bu + c$$

If we consider the iterative method

$$u_{k+1} = Bu_k + c, \quad \forall\ k \geq 0$$

we have

$$|u_k - u| \leq \|B^k\||u_0 - u|$$

The convergence speed of $u_k$ towards $u$ depends on the convergence speed of $B^k$ towards 0, so we need $\|B\| \leq 1$. Moreover, we have (Gelfand's formula)

$$\lim_{k\to\infty} \|B^k\|^{1/k} = \rho(B).$$

Hence the spectral radius $\rho(B)$ tells us about the speed of convergence of the iterative method.

# Why is spectral radius of B important?

$$x^1 = B x_0, \quad B \in \mathbb{R}^{n \times n}$$

$$x^2 = B x^1 = B^2 x_0$$

$$\vdots$$

$$x^k = B^k x_0$$

The eigenvectors of $B$ form a basis in $\mathbb{R}^n$, thus any vector in $\mathbb{R}^n$ can be expressed as a linear combination of these eigenvectors.

$$x_0 = \alpha_0 v_0 + \alpha_1 v_1 + \dots + \alpha_n v_n = \sum_{i=0}^{n} \alpha_i v_i, \text{ where } B v_i = \lambda_i v_i$$

$$\Rightarrow x^k = B^k x_0 = B^k \sum_{i=0}^{n} \alpha_i v_i = \sum_{i=0}^{n} \alpha_i \underbrace{B^k v_i}_{\lambda_i^k v_i} = \sum_{i=0}^{n} \alpha_i \lambda_i^k v_i$$

if $\max_i |\lambda_i| > 1$, then the iterative process will diverge!

# Geometrical interpretation

Eigen vectors only get scaled, not changed in direction!

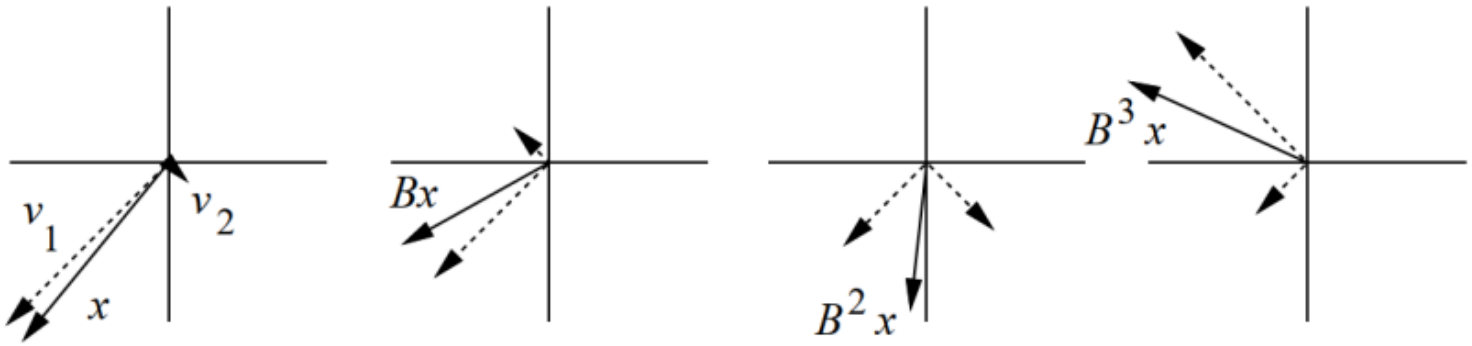



Figure 11: The vector $x$ (solid arrow) can be expressed as a linear combination of eigenvectors (dashed arrows), whose associated eigenvalues are $\lambda_1 = 0.7$ and $\lambda_2 = -2$. The effect of repeatedly applying $B$ to $x$ is best understood by examining the effect of $B$ on each eigenvector. When $B$ is repeatedly applied, one eigenvector converges to zero while the other diverges; hence, $B^i x$ also diverges.

Figure: From Shewchuk, J. R. (1994). An introduction to the conjugate gradient method without the agonizing pain.

# Another matrix decomposition

Given a linear system

$$Au = b,$$

we suppose that $A$ is invertible and that it can be written under the form

$$A = M - N$$

where $M$ and $N$ are two matrices with $M$ invertible.

We have

$$Au = b \iff Mu = Nu + b \iff u = M^{-1}Nu + M^{-1}b$$

If we set $B = M^{-1}N$ and $c = M^{-1}b$, we obtain $u = Bu + c$ and the iterative method reads

$$u_{k+1} = Bu_k + c = M^{-1}Nu_k + M^{-1}b$$

# Another matrix decomposition

## Remarks

- we do not compute $M^{-1}$ ! it is enough to solve at each iteration

$$Mu_{k+1} = Nu_k + b$$

- to this end we need to choose $M$ such that the system is easy to solve

# Towards a decomposition of A

Let

$$A = \begin{pmatrix} a_{1,1} & a_{1,2} & \cdots & \cdots & \cdots & \cdots & a_{1,n} \\ a_{2,1} & a_{2,2} & \ddots & & & & \vdots \\ \vdots & \ddots & \ddots & \ddots & & -F & \vdots \\ \vdots & & \ddots & D & \ddots & & \vdots \\ \vdots & -E & & \ddots & \ddots & \ddots & \vdots \\ \vdots & & & & \ddots & a_{n-1,n-1} & a_{n-1,n} \\ a_{n,1} & \cdots & \cdots & \cdots & \cdots & a_{n,n-1} & a_{n,n} \end{pmatrix}$$

$$A = D - E - F$$

$D$ diagonal matrix, $E$ lower triangular matrix, $F$ upper triangular matrix

We suppose $a_{i,i} \neq 0$ for all $i \in [\![1, n]\!]$

# Jacobi iterative method

The simplest decomposition is

$$M = D, \quad N = E + F$$

$$Au = b \Longleftrightarrow Du = (E + F)u + b \Longleftrightarrow u = D^{-1}(E + F)u + D^{-1}b$$

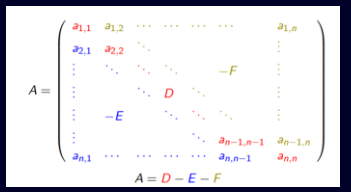
we obtain the Jacobi method

$$Du_{k+1} = (E + F)u_k + b \Longleftrightarrow u_{k+1} = D^{-1}(E + F)u_k + D^{-1}b$$

The Jacobi iteration matrix is

$$J = D^{-1}(E + F)$$

# Jacobi iterative method




## Pseudo code

$u^0$ given
For $k = 0$ to ... (stopping criterion)
  For $i = 1$ to $n$
    $u_i^{k+1} := \left( -\sum_{p \neq i} a_{ip} u_p^k + b_i \right) / a_{ii}$.

$[E+F]\{u^k\}$

$D^{-1}$

### Remarks

- we need to keep in memory all the $u_p^k$ to obtain $u_i^{k+1}$
- we can reduce the memory usage by replacing the computed $u_p^k$ by $u_p^{k+1}$ in the sum

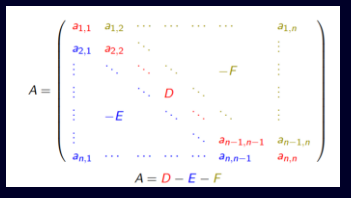
# Gauss Seidel algorithm

This gives the Gauss-Seidel algorithm

## Pseudo code

$$
\left[
\begin{array}{l}
u^0 \text{ given} \\
\text{For } k = 0 \text{ to } \ldots \text{ (stopping criterion)} \\
\quad \left[
\begin{array}{l}
\text{For } i = 1 \text{ to } n \\
u_i^{k+1} := \left( - \sum_{p<i} a_{ip} u_p^{k+1} - \sum_{p>i} a_{ip} u_p^k + b_i \right) / a_{ii}.
\end{array}
\right.
\end{array}
\right.
$$

# Gauss-Seidel iterative method




In its matrix form, we have

$$Du_{k+1} = Eu_{k+1} + Fu_k + b$$

which we rewrite as

$$(D - E)u_{k+1} = Fu_k + b \iff u_{k+1} = (D - E)^{-1}Fu_k + (D - E)^{-1}b$$

here we have

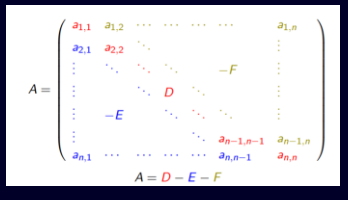
$$M = D - E, \quad N = F$$

($M$ is invertible since $a_{i,i} \neq 0$ for all $i \in [\![1, n]\!]$)

The iteration Gauss-Seidel matrix $\mathcal{L}_1$ is

$$\mathcal{L}_1 = (D - E)^{-1}F$$

# Relaxation method: Successive over-relaxation (SOR)




## Remarks

- If the Gauss-Seidel method converges, we can add a real parameter $\omega \neq 0$ such that

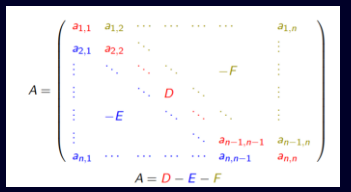
$$A = M - N = \left(\frac{D}{\omega} - E\right) - \left(\frac{1-\omega}{\omega}D + F\right)$$

- if the method converges $\rho(\mathcal{L}_1) < 1$, and by continuity of the spectral radius the iterative method must converge when $\omega$ is close to 1
- a similar approach could be used for any iterative method

The point-wise update is at the $k$-th iteration is

$$u_i^{k+1} = (1-\omega)u_i^k + \frac{\omega}{a_{ii}}\left(b_i - \sum_{j<i} a_{ij}u_j^{k+1} - \sum_{j>i} a_{ij}u_j^k\right), \quad i = 1, 2, \ldots, n.$$

# Relaxation method: Successive over-relaxation (SOR)




The point-wise update is at the $k$-th iteration is

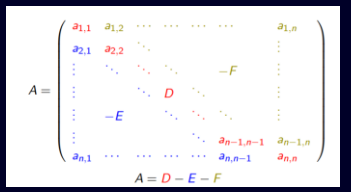
$$u_i^{k+1} = (1-\omega)u_i^k + \frac{\omega}{a_{ii}}\left(b_i - \sum_{j<i} a_{ij}u_j^{k+1} - \sum_{j>i} a_{ij}u_j^k\right), \quad i = 1, 2, \ldots, n.$$

- $\omega = 1$: Gauss - Seidel
- $\omega < 1$: Successive under-relaxation
- $\omega > 1$: successive over-relaxation (SOR)

$\omega \in ]0, 2[$

→ most common approach, gives more weight to the update

# Relaxation method: Successive over-relaxation (SOR)




The associated iterative method is

$$\left(\frac{D}{\omega} - E\right) u_{k+1} = \left(\frac{1-\omega}{\omega} D + F\right) u_k + b$$

The iterative matrix is called relaxation matrix $\mathcal{L}_\omega$

$$\mathcal{L}_\omega = \left(\frac{D}{\omega} - E\right)^{-1} \left(\frac{1-\omega}{\omega} D + F\right)$$

**Remark**

The relaxation method consists in finding

- an interval I $(0 \notin I)$ such that $\omega \in I \Rightarrow \rho(\mathcal{L}_\omega) < 1$
- an optimal relaxation parameter $\omega_0 \in I$ such that

$$\rho(\mathcal{L}_{\omega_0}) = \min_{\omega \in I} \rho(\mathcal{L}_\omega)$$

# Convergence of SOR

**Theorem: necessary condition for the convergence of the relaxation method**

for all $\omega \neq 0$, we have

$$\rho(\mathcal{L}_\omega) \geq |\omega - 1|$$

thus if $\omega \notin ]0, 2[$ the relaxation method does not converge.

**Theorem: sufficient convergence condition for the relaxation method**

If $A$ is a symmetric positive-definite matrix, the relaxation method converges for all $\omega \in ]0, 2[$. In particular the Gauss-Seidel method converges.

Remark: the theorem holds for hermitian matrices.

# Convergence of Gauss-Seidel and Jacobi

**Theorem**

If $A$ is strictly diagonal dominant

$$\forall i = 1, ..., N \qquad |a_{ii}| > \sum_{j \neq i} |a_{ij}|$$

then $A$ is invertible and the Gauss-Seidel and Jacobi methods converge.

# In general

**Remarks:**

- For many systems coming from discretization of PDEs, the Gauss-Seidel method converges faster than the Jacobi method
- For a large family of such systems, we can show that there exists a optimal parameter $\omega^\star$ for which the relaxation method is way more efficient: the number of required iterations for a given precision drops when $\omega \approx \omega^\star$

# Matrices of type “V”

Let us note

$$L = D^{-1}E, \quad U = D^{-1}F$$

hence

$$\begin{aligned} A &= D(I - L - U), \quad J = L + U \\ L_\omega &= (I - \omega L)^{-1}((1-\omega)I + \omega U). \end{aligned}$$

**Definition**

we say that $A$ if of type $(V)$, if for $\alpha \neq 0$, the eigenvalues of $J(\alpha) = \alpha L + \frac{1}{\alpha}U$ are independent of $\alpha$.

**Remarks**

- tridiagonal matrices are of type $(V)$
- many matrices form PDE discretization are of type $(V)$

# A few words about conditioning

**Conditioning** has a crucial role when solving linear systems. For a given induced matrix norm, it is defined as

$$\kappa(A) = \|A\|\|A^{-1}\|$$

## Forward error analysis

Let $A$ be invertible and $u$ and $u + \hat{u}$ be the solutions of the linear systems

$$Au = b, \quad A(u + \hat{u}) = b + \hat{b}$$

If $b \neq 0$ then the inequality

$$\frac{|\hat{u} - u|}{|u|} \leq \kappa(A) \frac{|\hat{b} - b|}{|b|}$$

holds and it is optimal.

# A few words about conditioning

Exercise 5

## Backward error analysis

Let $A$ be invertible and $u$ and $u + \tilde{u}$ be the solutions of the linear systems

$$Au = b, \quad (A + \tilde{A})(u + \tilde{u}) = b$$

If $b \neq 0$ then the inequality

$$\frac{|\tilde{u}|}{|u + \tilde{u}|} \leq \kappa(A) \frac{\|\tilde{A}\|}{\|A\|}$$

holds and it is optimal

If A is symmetric positive definite with eigenvalues $\lambda_1 \leq \cdots \leq \lambda_n$

$$\kappa_2(A) = \frac{\lambda_n}{\lambda_1}$$

For a more general matrix we use the singular values of $A$ to define $\kappa_2(A)$.
In practice, only the order of magnitude of $\kappa(A)$ matters.


# 6. Summary

# Summary

We have seen two families of methods for solving linear systems

**Direct methods :**

1. The modern form of Gaussian Elimination is called LU decomposition
2. A pivoting strategy is required for numerical stability
3. Cholesky decomposition is used for positive-definite matrices
4. Special algorithms are used for sparse matrices to reduce the computational cost

**Iterative methods :**

1. We have seen three types of fixed-point algorithms (Jacobi, Gauss-Seidel, SOR)
2. The convergence depends on the spectral radius of the matrix
3. They are advocated for very large systems, where direct methods become too costly